

U.S. Environmental Protection Agency

Upgrading MOBILE to Include Air Toxic Emission Factors Proposed MOBILE6.2 Project Description

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1. Introduction

OTAQ's Assessment and Modeling Center is undertaking a project to integrate the calculation of highway vehicle air toxic emission factors for benzene, 1,3-butadiene, formaldehyde, acetaldehyde, acrolein, MTBE and other hazardous air pollutants (HAPs) into the MOBILE6.X series of models. These emissions are currently estimated using a complicated set of tools that include six spreadsheets that contain a modified version of the EPA Complex Model, three Fortran programs, a Microsoft Access Database program and a modified version of MOBILE5 called MOBTOX. The rationale for developing a single software tool for estimating air toxic emissions is to simplify the modeling process for both in-house modeling efforts and external users. It will make the modeling process simpler for users who will be given a single, consistent interface for modeling functions, and it will avoid significant duplication of technical material between models. The development process also allows EPA to update the model to be based on final MOBILE6 parameters rather than a mix of the MOBILE5 framework and draft MOBILE6 parameters used in the current version of the MOBTOX5b model. Finally, combining the Air Toxic and the MOBILE models is a recommendation of *Modeling MOBILE SOURCE Emissions*, the National Academy of Science Research Council's review of MOBILE. We've determined, therefore, to pursue the option of integrating the disparate set of Air Toxic modeling tools into the MOBILE6.1 model and to call the product of this effort "MOBILE6.2."

Our objective is to quickly produce a MOBILE6.2 that includes all of the current Complex model algorithms and data, as well as any recent sulfur control measures. It will also integrate algorithms developed for light-duty vehicles with older control technologies not included in the EPA Complex model, as well as those developed for heavy-duty vehicles. The model will also allow for optional user input of alternative air toxic emission factors and air toxic ratios for all pollutant types. Based on stakeholder input, EPA has concluded that there is a need for improved air toxic emission modeling capability this year. Thus we have set a goal of developing a working in-house version of the MOBILE6.2 model no later than October, 2001, and a final version for release by January, 2002. This means that MOBILE6.2 must be limited to programming into the MOBILE6.1 model the existing air toxic algorithms and data, or making minor modifications to existing algorithms and data.

Fortunately, most of the required information is currently available in spreadsheets and technical documentation created as part of the RFG and other rulemaking efforts or in documentation for EPA's National Toxics Inventory. However, for a few pollutants, this type of information is not readily available, or the Agency is in the process of analyzing new data and revising current methods.

In these cases, the program will allow the user to enter his own emission factor or a ratio to VOC emission levels to calculate the particular air toxic pollutant.

The project is mostly a Fortran programming project. The project schedule does not allow time for major revisions or project expansion. Such new work would require a great deal of new vehicle testing, considerable new analysis, and extensive peer and stakeholder review. This type of additional work would push the project into a several year time frame.

Further improvements to the estimation of mobile source air toxic emissions will be made in the course of the longer term effort to produce an entire New Generation of mobile source air pollution Models (NGM). The NGM will implement the National Academy of Science recommendations, will be based on an extensive database of emission measurements made during actual operation of in-use vehicles and will provide a framework for allocating emission estimates to much smaller geographic areas and time periods.

The following sections describe in more detail what will, and will not, be updated in MOBILE6.2.

2. What Features Will be Added to MOBILE6.2

- 2.1 The basic algorithms and data found in the current version of EPA's Modified Complex Model will be added to the MOBILE6.1 program. This includes the basic algorithms for calculating exhaust and evaporative air toxic emissions on Tier0 vehicles (Basic Complex Model).
- 2.2 Additional new algorithms and data from MOBTOX5b and the documentation for National Toxics Inventory will be added. This includes calculation of air toxic emission from pre-1981 model year vehicles and diesel vehicles, calculation of air toxic emissions from LEV and later vehicles, the effect of recent fuel sulfur control regulations and new emission standards for cars and trucks, the calculation of MTBE emission factors, and the calculation of acrolein. All of these algorithms and data have been peer reviewed, thoroughly documented, and have been part of the MOBTOX model process. However, they were not part of the original Complex model.
- 2.3 It is anticipated that the MOBILE6.2 model will add or possibly modify the following fuel input parameters to the MOBILE6.1 structure. These fuel related parameters are necessary in-order for the purposes of air toxic emission modeling.

Oxygen (wt%), E200(%), E300(%), Aromatic(vol%), Olefin(vol%), Benzene(vol%), Fuel Oxygenate Type(MTBE, ETBE, Ethanol, Tame, etc.)

All of these inputs will be converted to the MOBILE6 Command input structure rather than the old style MOBILE5 input structure used in the existing MOBTOX model. The inputs

of Sulfur(ppm) and RVP(psi) are required for the Air Toxic Emission calculation, but will not be modified in the MOBILE6.2 update.

2.4 MOBILE6.2 will allow the user to calculate emission factors in grams per mile for up to 20 additional pollutants by having the user supply the following information:

- The air toxic pollutant name.
- Whether the air toxic pollutant is emitted in the exhaust or evaporative modes, and if so to supply toxic/VOC emission ratios for the pollutant for each MOBILE6 vehicle class. Different ratios can be supplied for different model year ranges, and vehicle classes.
- To calculate exhaust emission rates of the pollutant the user will be allowed to supply any one combination of the following by MOBILE6 vehicle class and model year range:
 - Toxic/VOC emission ratio
 - Toxic/PM emission ratio
 - Basic emission rates for the exhaust emissions of the pollutant. These will be in the form of a zero mile emission rate in grams per mile, plus a linear deterioration factor in units of grams per mile per 10,000 miles of vehicle travel.

Note that the distinction by MOBILE6 vehicle class allows separate emission factors to be modeled for gasoline versus diesel fueled vehicles. However, modeling of other fuel properties for these “additional pollutants” would have to be done with multiple input files and model runs.

EPA will supply input files of default information to estimate the emissions of various additional air toxic pollutants as the information becomes available, including information that becomes available after the release of MOBILE6.2.

MOBILE6.2 will calculate default values and allow alternative user emission factors in units of grams per mile for the following SIX principal air toxic pollutants.

Acetaldehyde
Formaldehyde
1,3 Butadiene
Exhaust and Evaporative Benzene
Exhaust and Evaporative MTBE
Acrolein

Because the new model will be based on MOBILE6 VOC emission factors, and in a few cases, particulate emission factors, the final air toxic emission results will NOT necessarily be equal to the existing MOBTOX emission factor results which were based on draft MOBILE6 parameters integrated into a MOBILE5 framework.

The MOBILE6.2 model will also allow the user the flexibility to model the following pollutants and any other user defined pollutants. The program will be general in nature, and allow either the 'ratio' method or the 'emission factor' method for these pollutants. Tentatively, it will not provide default, built-in emission factors for these pollutants. They are listed here as an example of the particular type of air toxic pollutant that may be modeled.

- Ethylbenzene
- Naphthalene
- n-Hexane
- Styrene
- Toluene
- Xylene
- Dioxin/Furans
- Nickel Compounds
- Arsenic Compounds
- Manganese Compounds
- Chromium Compounds
- Mercury Compounds
- Polycyclic Organic Matter (POM) - This contains up to 16 separate compounds

- 2.5 The exhaust and evaporative air toxic emissions from Zero Emission Vehicles (ZEVs) will be considered to be zero.
- 2.6 Since no data are available, the exhaust and evaporative air toxic emissions from Natural Gas Fueled Vehicles will not be produced as a default. Instead, the user will have to supply their own air toxic emission factors or ratios to model these vehicle types.
- 2.7 MOBILE6.1 input data will be used wherever it applies to Air Toxic emission calculations. This type of data includes vehicle registration, diesel fraction, and mileage accumulation information.
- 2.8 The MOBILE6.1 Database style of reporting emission results will be used in the MOBILE6.2 model. The only substantial change will be adding the Six air toxic pollutants to the current list of pollutants that include HC, CO, NOX, particulate components, etc. Air Toxic emission results from alternate pollutants supplied by the user will also be reported in the database output. MOBILE6.2 will also produce an additional descriptive output that provides composite air toxic emission results for all pollutants. This air toxic emission output will remain separate from the two output reports currently produced by MOBILE6.1.

- 2.9 The MOBILE6.2 model will contain to a limited extent new air toxic emission factors for LEV and Tier2 vehicles. This means that the air toxic emission / VOC emission ratio are assumed to be the same for LEV / Tier2 as for Tier0. This assumption was necessary because of inadequate data to properly define an alternate relationship for post Tier0 vehicles. However, a limited sample of LEV speciation data did suggest that this assumption is reasonable.
- 2.10 A single, consolidated MOBILE6.2 User's Guide will be produced.
- 2.11 Guidance for the use of MOBILE6.2 will be developed, and default emission factors or ratios for some air toxic pollutants may be supplied when possible.
- 2.12 The FUEL PROGRAM command in MOBILE6.0 will be retained for backward compatibility of the program, but will not be allowed in conjunction with estimation of the air toxic emissions.

3. What Features Will NOT be Changed or Added to MOBILE6.2

- 3.1 The MOBILE6.2 model will produce identical HC, CO and NO_x emission factors as the final release of MOBILE6.0. In addition, we are planning on keeping the MOBILE6 input command structure backward compatible with respect to HC, CO and NO_x emission modeling.
- 3.2 The MOBILE6.2 model development process will not consider new analysis or data to update the basic functional relationship of the Primary Six air toxic pollutants to fuel properties. However, some new analysis may be done to provide guidance to users who wish to enter alternate emission factors or ratios for other air toxic pollutants. The intention of this task is to produce a more useable model that reflects the existing EPA Complex model algorithms and the peer reviewed data and analytical additions to it that were part of the MOBILE5 MOBTOX process.
- 3.3 The MOBILE6.2 model will include air toxic estimates for all 28 MOBILE6 vehicle types (light and heavy duty and gasoline and diesel vehicles). However, emission factors for all vehicles and particularly the diesel vehicles are based on a limited amount of data. This limited amount of diesel data will not be updated from that currently found in the MOBTOX process.
- 3.4 The MOBILE6.2 model will probably not contain special air toxic emission ratios to model the effects of the 2007 Heavy-duty vehicle regulations (some consideration for the effect of exhaust traps may be considered, though). However, because the MOBILE6.0 model contains new VOC emission factors for these vehicles, and the MOBILE6.1 program will allow lower diesel fuel sulfur emissions to be entered, the final air toxic emission results for diesels will model some effects of the 2007 regulation and will be different than those reported by the MOBTOX model.